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The Continuous Flow Analyzer Automation System Part II -- User's Guide

Cincinnati Univ. Computing Center, OH

Prepared for

Environmental Monitoring and Support Lab.
Cincinnati, OH

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THE CONTINUOUS FLOW ANALYZER AUTOMATION SYSTEM
PART II -- USER'S GUIDE

by

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Contract No. GS-05S-10458

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This publication contains the user's guide to the EPA Continuous Flow Analyzer Automation System. This system can receive lists of samples from the Sample File Control (SFC) System and return the measured concentrations to that system or the automation system can operate independently of SFC and only output the final results to a hardcopy unit. It is capable of interfacing with three continuous flow analyzer detectors simultaneously. It incorporates the following major features: 1) baseline interpolation between blanks, 2) multi-point calibration using first, second, or third degree regression or linear interpolation, 3) timely quality control assessments for spiked samples, duplicates, laboratory control standards, reagent blanks, and instrument check standards, 4) reagent blank subtraction, and 5) plotting of calibration curves and raw data peaks.

This doucment contains detailed descriptions and examples of the features of the system, as they appear to the user.

Two related publications are titled, "The Continuous Flow Analyzer Automation System, Part I -- Functional Specifications," and "The Continuous Flow Analyzer Automation System, Part III -- Program Documentation."

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati, conducts research to:

- Develop and evaluate techniques to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.
- Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water, and to determine the responses of aquatic organisms to water quality.
- Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.
- Develop and operate a computerized system for instrument automation leading to improved data collection, analysis, and quality control.

This report was developed in the Advanced Instrumentation Section of the Environmental Monitoring and Support Laboratory in the interest of advancing laboratory techniques and quality control through computerization.

Robert L. Booth
Acting Director
Environmental Monitoring and Support
Laboratory - Cincinnati

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ABSTRACT

This publication contains the user's guide to the EPA Continuous Flow Analyzer Automation System. This system can receive lists of samples from the Sample File Control System and return the measured concentrations to that system. It is capable of interfacing with three continuous flow analyzer detectors simultaneously. It incorporates the following major features: 1) baseline interpolation between blanks, 2) multi-point calibration using first, second, or third degree regression or linear interpolation, 3) timely quality control assessments for spiked samples, duplicates, laboratory control standards, reagent blanks, and instrument check standards, 4) reagent blank subtraction, and 5) plotting of calibration curves and raw data peaks.

The programs of this system are written in Data General Extended BASIC, Revision 4.3, as enhanced for multi-user, real-time data acquisition. They run in a Data General Nova 840 minicomputer under the operating system RDOS, Revision 6.2.

Two related publications are titled, "The Continuous Flow Analyzer Automation System, Part I -- Functional Specifications" and "The Continuous Flow Analyzer Automation System, Part III -- Program Documentation."

This document contains detailed descriptions and examples of the features of the system, as they appear to the user.

This report was submitted in partial fulfillment of Task No. 80-07 of Contract No. GS-05S-10458 by the University of Cincinnati Computer Center under the sponsorship of the U. S. Environmental Protection Agency. It covers work done between April 16, 1980, and May 1, 1980.

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SECTION 1

INTRODUCTION

The Continuous Flow Analyzer (CFA) Automation System is a set of computer programs totaling over 6800 statements. The system enables you to collect and process data from up to three continuous flow analyzer detectors simultaneously. It synchronizes itself with the automatic samplers, determines peak heights, performs calibration, and calculates concentrations. It accepts lists of samples from the Sample File Control System and reports results back to that system. It provides quality control assessments for spiked samples, duplicate samples, laboratory control standards, reagent blanks, and instrument check standards. It takes dilution factors into account and allows for the dilution and remeasurement of offscale samples. It interpolates the baseline between blanks. It allows for manipulation of the calibration equations, and subtraction of reagent blanks. It can determine calculated concentrations, as in the case of the "nitrate-nitrite minus nitrite" method for measuring nitrate. It is capable of plotting raw data and calibration curves on a graphics terminal. Also, all of the features of the system are designed to allow it to be operated in an unattended mode.

The CFA System is intended to be as self-explanatory and mistake-proof as possible. Every time the system confronts you with a "menu" of options, the first option is to get an explanation of the other options. If you enter an unreasonable answer to any question, the system tells you so, and it restates the question. During the manipulation of data after it has been acquired, the system makes it impossible for you to destroy your raw data. Therefore, if you do make a serious mistake, you can always revert to your raw data and manipulate it differently, even after a final report has been printed. In any case, there is no way that you can damage the computer or its programs by experimenting with the CFA Automation System.

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SECTION 2

SIGNING ON TO THE SYSTEM

The CFA Automation System runs on a Nova 840 minicomputer. To sign on to the system, you must use a terminal which is properly connected to the Nova and set for full duplex, on line, no parity, and 300 baud (or a higher baud rate, if permitted by the Nova system manager).

To get the attention of the Nova, press the ESCAPE key once. (Some Tektronix terminals do not have an ESCAPE key. On such terminals, hold down the CONTROL and SHIFT keys, and press the K key.) If the Nova system is already servicing as many users as it can, it responds with a message to that effect, but normally it asks for your "account ID." The Nova system manager should have assigned you a pair of account ID's for each one of the analytes that you normally measure. Type the appropriate account ID, and press the RETURN key. The account ID is not displayed on your terminal as you type it.

Next, the Nova system usually prints some message of the day, and it then automatically transfers control of the computer to the programs you need to use. This feature protects the integrity of the system by making it impossible for any user to change the programs or data files. (If you want to write your own BASIC programs, you have to sign on to the Nova under a different account ID.)

At this point, there are three possible occurrences: 1) If you are involved with Sample File Control, you are confronted with the Sample File Control master command menu. Using features of that system, you must create a "run file," which is a list of the samples you intend to measure, drawn from the Sample File Control backlog, as described in the document "User's Guide for the Sample File Control System in the Nova 840." When you have created your run file, use the AUTORUN option of the Sample File Control master command menu to enter the CFA Automation System. 2) If you are not involved with Sample File Control, but your Nova system manager prefers that all of the Nova users pass through the Sample File Control master command menu, you are confronted with that menu. Simply choose the AUTORUN option of the menu to immediately enter the CFA Automation System. 3) If neither you nor your system manager is involved with Sample File Control, you are not confronted with that system's master command menu, but rather you enter the CFA Automation System immediately after the message of the day has been printed.

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In any case, when you enter the CFA System, you are confronted with the CFA master command menu.

The second account ID for each analyte allows you to sign on to two terminals at the same time. When you use the second account ID, however, you do not see the message of the day, but rather you enter a program which allows you to do nothing but plot your calibration curves.

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SECTION 3

GENERAL PRINCIPLES OF THE SYSTEM

There are several general principles for using the CFA System which apply to all of its options. The first of these is that any time you answer a question, you must follow your answer with a RETURN, to indicate to the computer that you are done typing.

If you make a typing error and notice it before you press RETURN, you can correct it. Pressing the RUBOUT key (the DELETE key on some terminals) eliminates the last character you typed. Typing a backslash (\) eliminates your entire entry.

It is never appropriate to type a comma in the CFA System. For example, to enter the number one million, you must type "1000000." Due to a limitation of the BASIC language in the Nova, if you type a comma as part of a word or number, the comma and all of the characters following it will be truncated.

Whenever the CFA System wants you to type information, it cues you with two "greater than" symbols. For example:

NAME OF ANALYTE >>

If there is a limited number of acceptable responses, the system lists those responses within the question. For example:

IS VOLUME OF SPIKING SOLUTION SIGNIFICANT ([N],Y) >>

The response in square brackets is always the response which the system uses by default if you simply press RETURN without typing an answer. An H in square brackets always stands for "help." If you type the H or simply press RETURN, the system will help you by briefly explaining the other options.

For some questions, there is an unlimited number of possible responses, but the system can suggest your probable response, based on how you answered the question the last time you came to it. For example:

TIME BETWEEN PEAKS, IN SECONDS ([120],---) >>

In this case, the square brackets indicate that pressing RETURN is the same as typing "120", and the "---" symbol indicates that you may instead type

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any of an unlimited set of other responses.

If you press the ESCAPE key (or the Tektronix CONTROL, SHIFT, K) at any time while you are using the CFA System, you are returned to the CFA master command menu.

At many points in the CFA System, the Nova does thousands of operations for every one that you do, while at the same time it is also servicing several other users. Consequently, slight hesitations are perfectly normal. If the system appears to have stopped working, be patient for at least a full minute, and the system will probably resume normal operation. This caution also applies when you press the ESCAPE key. When the system is interrupted by the ESCAPE key, it often must "tidy up" quite a few internal problems before it can offer you the full choice of its master command menu. Thus, when you use the ESCAPE key, press it once firmly, and then be patient for the few moments that it may take the system to respond.

During a few very lengthy operations, the system lets you know that it is still active by occasionally typing another period onto the end of an ellipsis. For example:

THE FINAL RESULTS ARE BEING CALCULATED.....

If you discover an error in the CFA System, or if you wish to add an enhancement to it, do not attempt to alter the programs yourself. Any errors should be brought to the attention of the Advanced Instrumentation Section, together with enough details of the circumstances so that the error can be reproduced. Any error will be corrected, and the amended programs will be distributed to all users immediately. Similarly, enhancement requests should be directed to the Advanced Instrumentation Section. Enhancements which would be of significant value will be included in future releases of the system, as funding and person power permit.

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SECTION 4

THE MASTER COMMAND MENU

When you first enter the CFA Automation System, you are confronted with the CFA master command menu. To choose from this menu intelligently, you must understand the flow of the system as a whole. Figure 1 is a functional flowchart which shows the eight distinct sections of the CFA System. (There are actually 21 computer programs in the system. For a flowchart showing individual programs, see the book, "Program Documentation for the Continuous Flow Analyzer Automation System.") Figure 2 shows how the master command menu appears on the terminal. As you can see in Figure 1, the master command menu simply allows you to jump directly to any of the major sections of the system, except for option P which is arrived at by logging on under your second account ID.

If you choose option G, the system allows you to generate a non-Sample File Control run file. A run file is a list of the samples in the order in which they are to be measured. If you are involved with Sample File Control, you will never use option G, since you must create your run files using the Sample File Control System before you enter the CFA System. After a non-Sample File Control run file has been created, the system returns to the CFA master command menu.

Option S of the master command menu is used to start an automated run. It is impossible to use option S until you have created a run file. Starting an automated run involves four tasks: 1) the run file is assimilated into the automation system, 2) you are asked to input dilution and spiking information, 3) the sample wheel pattern can be printed, and 4) you are asked to input the automation parameters (the time between peaks, the detection limits, etc.). After you have completed all of these tasks, the system automatically selects option A for you.

Under option A, the computer programs acquire data and print the progress report. Obviously, the system cannot permit you to use option A until after you have finished all the tasks under option S. Option A is provided in the master command menu so that if you need to abort an automated run, it is possible to restart the run without re-answering all of the questions in the first section. When the data has been acquired and displayed on the progress report for the entire batch, the system automatically advances to option M.

Under option M, the programs manipulate the data. That is, the baseline is interpolated between the blanks. The final calibration equations are

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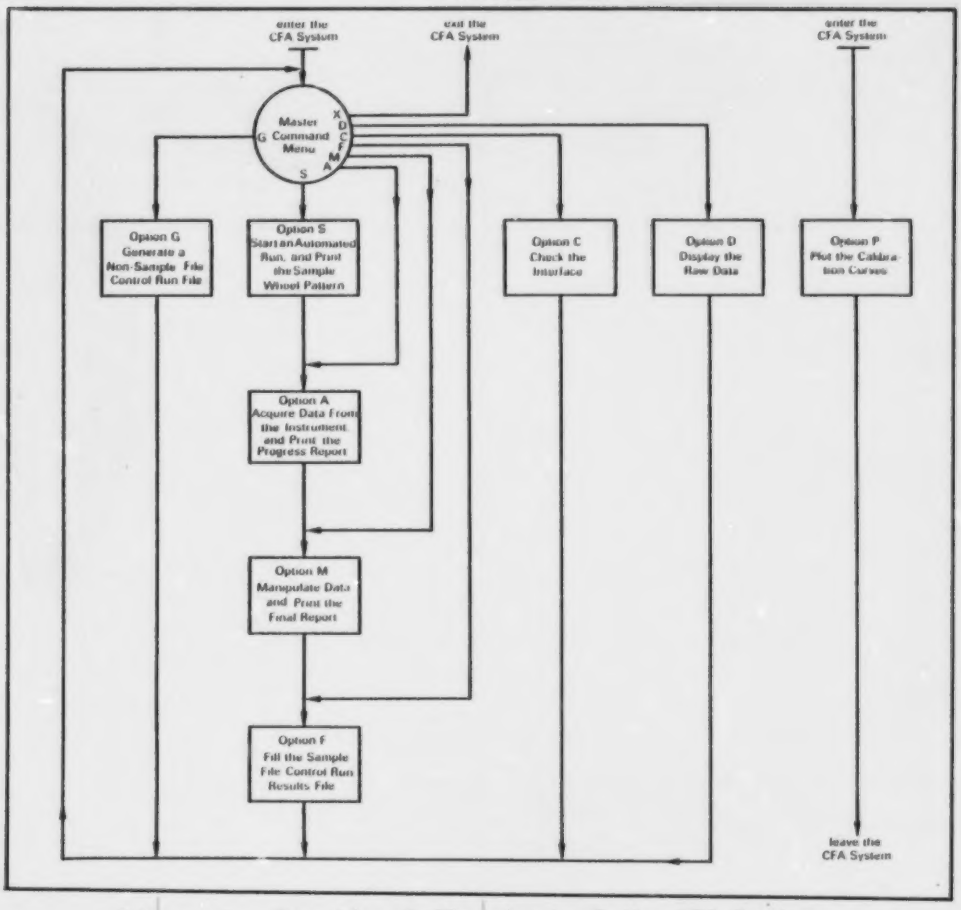
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Master Command Menu
G
S
X
D
C
F
M
A
Option G Generate a Non-Sample File Control Run File
Option S Start an Automated Run, and Print the Sample Wheel Pattern
Option C Check the Interface
Option D Display the Raw Data
Option P Plot the Calibration Curves
Option A Acquire Data From the Instrument and Print the Progress Report
Option M Manipulate Data and Print the Final Report
Option F Fill the Sample File Control Run Results File
leave the CFA System

Figure 1. Functional Flowchart of the CFA System.

```
H = HELP
G = GENERATE A NON-SFC RUN FILE
S = START OR RESTART AN AUTOMATED RUN FROM THE POINT OF ASSIMILATING
    A RUN FILE
A = ACQUIRE RAW DATA;  RESTART AN AUTOMATED RUN FROM THE POINT OF
    ESTABLISHING FULL SCALE AND BASELINE
M = MANIPULATE DATA AND GET A FINAL REPORT FOR A BATCH WHICH HAS ALREADY
    BEEN PROCESSED, OR FOR A BATCH WHICH HAS BEEN ABORTED
F = FILL THE SFC RUN RESULTS FILE FOR A BATCH FOR WHICH A FINAL
    REPORT HAS BEEN PRINTED BUT FOR WHICH THE RUN RESULTS FILE HAS NOT
    BEEN FILLED PREVIOUSLY
C = CHECK THE INTERFACE HARDWARE
D = DISPLAY THE RAW DATA
X = EXIT THE CFA AUTOMATION SYSTEM (THIS IS THE DEFAULT ANSWER IF THERE
    IS NO RESPONSE IN 10 MINUTES)

CFA MASTER COMMAND ([H],G,S,A,M,F,C,D,X) ))
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Figure 2. The Master Command Menu.

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developed, and it is possible to manipulate, report, and/or plot the calibration information. Reagent blanks can be subtracted, and the final reports are printed. The system cannot allow you to use option M until you have at least passed the point of the initial calibration under option A. There are two logical reasons for picking option M from the master command menu: 1) to remanipulate data to improve your results by recalibration or other techniques, and 2) to manipulate and report the data for an automated run which was aborted before it came to the end of the batch of samples. When the functions under option M have been completed, the system branches back to the master command menu if you began with a non-Sample File Control run file, or it advances to option F if you began with a run file produced by the Sample File Control System.

The purpose of option F is to have the programs fill the Sample File Control run results file. A run results file is the list of all of the samples which were measured, together with their measured concentrations. The system cannot permit you to use option F of the master command menu unless you have used a Sample File Control run file and you have completed all of the functions under option M. There is only one logical reason for picking option F at the master command menu level. When you first arrive at option F, if you are not ready to approve the results for transmission to Sample File Control, you can sign off from the computer, study the final report, and then return through option F to fill the run results file. This procedure is especially useful for unattended runs which end during the night. After the run results file has been filled, the system returns to the master command menu.

Option C allows you to check the interface hardware.

Option D is used to display the raw data. The system cannot allow you to use option D until you have measured at least one sample. After completing either option C or option D, the system returns to the master command menu.

Option P is different from all of the others in that it cannot be reached from the master command menu. Its primary purpose is to plot the calibration curves while data acquisition is in progress. Therefore, option P must be reached by using a second terminal to log on to the Nova, using the second account ID which your system manager has provided for each analyte. When calibration curve plotting has been completed, you are automatically logged off from the computer.

If you press the ESCAPE key at any point in the CFA System, you return to the CFA master command menu. The only exception is in option P where pressing the ESCAPE key causes you to be logged off from the computer entirely.

The only way to leave the main CFA System is to use the X option of the master command menu to exit back to where you began. That is, if you entered the CFA System from the Sample File Control System, the X option sends you back to Sample File Control. Alternatively, if you entered the CFA System directly when you logged on to the computer, then option X causes you to be logged off.

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SECTION 5

GENERATING A NON-SAMPLE FILE CONTROL RUN FILE

A "run file" is the computer's list of samples to be measured, including all standards, unknowns, quality control items, and blanks. If you are involved with the Sample File Control data base, you must generate a run file before you enter the CFA Automation System. However, if you are not involved with Sample File Control, using option G of the CFA master command menu enables you to generate a run file.

The first time that you generate a run file for an analyte or set of analytes, you must answer quite a few questions to create the "templates" and to establish the quality control limits. A template is a pattern for how the samples are to be arranged in the sample wheel. Once the templates and quality control limits have been established for an analyte, you can create subsequent run files by supplying as few as five very terse responses. Having a separate account ID for each of the analytes you regularly measure enables you to store all of the analyte-specific data that you need.

5.1 TEMPLATES

When you use the G option of the master command menu, you are confronted with the question:

TEMPLATES ([H],A,D,G,) >>

where H, as always, means "help." The letter A means "accept the existing templates," D means "display the existing templates," and G means "generate new templates." The very first time you use the system, it skips this question and forces you to generate new templates. To begin that process, the system first asks for the number of analytes (at most three) and the names of the analytes (at most seven characters in a name). You may wish to use the Sample File Control "parameter-method codes" as the names of the analytes, although any unique names are acceptable. There are actually four templates which must be generated, although the system automatically does all of the work for generating two of them and most of the work for a third one.

The Calibration Template

The calibration template is used to form the first fragment of the sample wheel pattern. It always consists of three timing set standards, two

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instrument blanks, and the calibration standards. Timing set standards are samples of known concentration used by the system to synchronize itself with the automatic sampler. Since there are always three set standards and two blanks, the system automatically generates the first five positions of the calibration template. The information you must supply is the number of calibration standards and the prepared concentration of each analyte in each calibration standard. The concentrations of the standards should be entered in the default unit for the method, that is, the unit prescribed by the methods manual.

The Samples Template

The samples template is the series of unknowns and quality control items which is used repeatedly to form the bulk of the sample wheel pattern. To get the information it needs to form the samples template, the system prompts:

```
GENERATE SAMPLE TEMPLATE USING  [H],U,F,D,B,L,C,R,X
POSITION   1 >>
```

The letter U stands for "unknown." If you type U, the system asks for the number of consecutive unknowns, and it adds them to the template. The letter F stands for "spike." (The letter F is used to be consistent with other automation systems which use S to mean "standard." The meaning of F can be recalled by associating it with the formal name "laboratory spike final concentration.") For a spike, the system also asks for the template position of the corresponding unknown. The letter D stands for "duplicate." For a duplicate, the system also asks for the template position of the corresponding unknown. The letter B stands for "instrument blank." If you type B, the system asks for the number of consecutive blanks. The letter L stands for "laboratory control standard." If you type L, the system asks for the prepared concentration of each analyte in the control standard. For a laboratory control standard, any concentrations may be used. The letter C stands for "instrument check standard." If you type C, the system also asks for the prepared concentrations of the analytes; these must match one of the calibration standards exactly. The letter R stands for "reagent blank." The letter X is used to signify the end of the template.

The Leftover Unknowns Template

The leftover unknowns template is used to avoid the problems which would occur if the system tried to use part of a samples template to place the last few unknowns into the sample wheel pattern. The leftover unknowns template simply represents a wheel position for one unknown with no associated quality control items. This template is generated automatically by the system without human interaction. (Refer to Section 5.3 for further explanation.)

The Trailing Blanks Template

For this system, every sample wheel pattern must end with four blanks,

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and therefore the system automatically generates the trailing blanks template without human intervention.

When templates have been generated, the system returns to the question:

TEMPLATES ([H],A,D,G,) >>

If you choose the "display" option, the calibration and samples templates are printed on the terminal, as shown in Figure 3. The system then returns to the same templates question. When you choose the "accept" option, you advance into the next task.

5.2 QUALITY CONTROL LIMITS

When you have accepted your templates, the system asks:

QC LIMITS ([H],A,D,G,) >>

where the options once again are to accept, display, or generate quality control limits. The first time you use the system, it skips this question and forces you to generate quality control limits. For each analyte, you must supply the quality control limits for spiked samples, laboratory control standards, reagent blanks, and duplicates, even if you do not have such items in your templates.

Spiked Samples

The values which you must supply for spiked samples are the mean percent recovery and sigma (the standard deviation of the percent recoveries). The system establishes the upper and lower warning limits as the mean percent recovery, plus and minus two times sigma. It establishes the upper and lower control limits as the mean percent recovery, plus and minus three times sigma.

Laboratory Control Standards

The values to be typed and the final form of the control limits for laboratory control standards are identical to those for spiked samples.

Reagent Blanks

The values to be typed and the final form of the control limits for reagent blanks are the same as those for spiked samples, except that they are expressed in the default concentration units for the method, rather than in percent recoveries.

Duplicates

The control limits for duplicates are entirely different from those of the other quality control items. The values that the system asks for are C and D, which are coefficients of the equation:

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C-A-L-I-B-R-A-T-I-O-N T-E-M-P-L-A-T-E

TEMPLATE POSITION	SAMPLE TYPE		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
001	SET STND				
002	SET STND				
003	SET STND				
004	BLANK				
005	BLANK				
006	CAL STND	TCONC:	30.000	15.000	20.000
007	CAL STND	TCONC:	60.000	30.000	40.000
008	CAL STND	TCONC:	90.000	45.000	60.000

S-A-M-P-L-E T-E-M-P-L-A-T-E

TEMPLATE POSITION	SAMPLE TYPE		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
001	BLANK				
002	BLANK				
003	UNKNOWN				
004	UNKNOWN				
005	SPIKE OF 004				
006	DUPE OF 004				
007	CONTROL STND	LCT:	45.000	22.500	30.000
008	CHECK STND	CONC:	60.000	30.000	40.000
009	REAGENT BLNK				

Figure 3. Calibration and Samples Templates.

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$$\text{CRITICAL RANGE} = (A\bar{X})^3 + (B\bar{X})^2 + (C\bar{X}) + (D)$$

where the "critical range" is the greatest allowable difference between duplicates and X is the average concentration of a pair of duplicates. The coefficients A and B are always zero, but you must supply C and D.

When you have generated your quality control limits, the system returns to the question:

QC LIMITS ([H],A,D,G,) >>

If you choose to "display" the limits, the system provides a report such as that shown in Figure 4. After the limits have been printed, the system returns to the QC limits question. When you accept the limits, the system advances to the next section.

5.3 SAMPLE ID NUMBERS

After templates and quality control limits have been generated and accepted, the system asks:

SPECIFY ID NUMBERS FOR THE UNKNOWNS;
TYPE 0 (ZERO) AS AN ID TO END THE LIST

FIRST ID >>
LAST ID >>

This allows flexibility in the ID numbers while providing for quick entry of them. For example, if you wanted ID numbers ranging from 1 to 123, you would simply type those numbers as the first and last ID's, and then type a zero when the system asked for another first ID. Or you could create ID numbers in several groups (for example 1 to 45, 56 to 75, and 103 to 122), and then type a zero as an ID number. At the other extreme, you could enter each ID number individually by using each number as the first and last ID of a series.

When you type a zero as an ID, the system begins to assemble the run file. It first uses the calibration template to start the sample wheel pattern. It then uses the samples template repeatedly to build the sample wheel pattern until there are not enough unknowns left to fill one complete samples template. Then it uses the leftover unknowns template to enter the remaining unknowns into the sample wheel pattern, and finally it adds the trailing blanks template to the end of the batch of samples.

When the run file is complete, the system returns to its master command menu.

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Q-C L-I-M-I-T-S

LIMITS FOR 6210001:

SPIKED SAMPLES:
UCL = 115.000%
UWL = 110.000%
AVE = 100.000%
LWL = 90.000%
LCL = 85.000%

LABORATORY CONTROL STANDARDS:
UCL = 115.000%
UWL = 110.000%
AVE = 100.000%
LWL = 90.000%
LCL = 85.000%

REAGENT BLANKS:
UCL = 15.000
UWL = 10.000
AVE = 0.000
LWL = -10.000
LCL = -15.000

DUPLICATES:
A = 0.000
B = 0.000
C = 0.150
D = 0.000

LIMITS FOR 6220001:

SPIKED SAMPLES:
UCL = 115.000%
UWL = 110.000%
AVE = 100.000%
LWL = 90.000%
LCL = 85.000%

LABORATORY CONTROL STANDARDS:
UCL = 115.000%
UWL = 110.000%
AVE = 100.000%
LWL = 90.000%
LCL = 85.000%

REAGENT BLANKS:
UCL = 15.000
UWL = 10.000
AVE = 0.000
LWL = -10.000
LCL = -15.000

DUPLICATES:
A = 0.000
B = 0.000
C = 0.150
D = 0.000

Figure 4. Quality Control Limits Report.

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SECTION 6

STARTING AN AUTOMATED RUN

Starting an automated run involves six major steps: 1) assimilating a run file, 2) providing dilution information, 3) providing spiked sample information, 4) allowing for extra repeat positions, 5) printing the sample wheel pattern, and 6) providing values for the automation parameters.

6.1 ASSIMILATING A RUN FILE

When the system assimilates a run file, it copies from the run file all of the information that it needs, and at the same time, it checks to be sure that the sample wheel pattern is acceptable. Non-Sample File Control run files generated by this system are always in acceptable form, but the Sample File Control System is flexible enough to generate run files for other automation systems, and is therefore flexible enough to allow you to produce a run file which is unacceptable to this system. When the CFA Automation System assimilates a run file, it rejects the file if it does not meet the following specifications: 1) The run file must deal with one, two, or three analytes. 3) The run file must begin with three timing set standards, two blanks, and all of the calibration standards, in that order. 3) The run file must end with four instrument blanks. 4) The prepared concentrations of the analytes in every instrument check standard must match those of a calibration standard exactly.

As the system assimilates a run file, it prints a list of the sample wheel positions of the unknowns. This list is essential for the next task.

6.2 PROVIDING DILUTION INFORMATION

After assimilating a run file, the system prompts:

```
ANY DILUTIONS ([N],Y) >>
```

If you answer Y (yes) to that question, the system asks:

```
SPECIFY WHEEL POSITIONS OF UNKNOWNS TO BE DILUTED;
TYPE 0 (ZERO) AS A WHEEL POSITION TO END THE LIST

    FIRST POSITION >>
    LAST POSITION >>
    SAMPLE VOLUME IN ML >>
    DILUTION WATER VOLUME IN ML >>
```

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You may enter dilution information for the whole batch at once, or for groups of samples within the batch, or for individual unknowns by typing the proper sample wheel positions as the first and last positions. The sample wheel positions of the unknowns can be found on the list printed during the assimilation of the run file. Any time that a dilution is specified for an unknown, any spike or duplicate of that unknown is automatically assigned the same dilution factor, even if the spike or duplicate is not within the range of the specified first and last wheel positions. No samples other than unknowns, spikes, and duplicates are ever assigned dilution factors, even if they happen to be within the range of the specified first and last wheel positions. When you type a zero as a wheel position, the system advances to the next section.

6.3 PROVIDING SPIKED SAMPLE INFORMATION

After any dilution information has been entered, the system prints a list of the sample wheel positions of the spiked samples, if any. If there are spiked samples in the batch, the system asks:

```
IS VOLUME OF SPIKING SOLUTION SIGNIFICANT ([N],Y) >>
```

The volume of the spiking solution is significant and must be taken into account unless you perform spiking with a very concentrated solution using a micropipette.

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If the volume of your spiking solution is significant, the system asks:

```
SPECIFY WHEEL POSITIONS OF SPIKES TO WHICH DATA APPLIES;
TYPE 0 (ZERO) AS A WHEEL POSITION TO END THE LIST

    FIRST POSITION >>
    LAST POSITION >>
    SAMPLE VOLUME IN ML >>
    CONCENTRATION OF SPIKING SOLUTION IN DEFAULT UNITS:*
         6210001 >>
         6220001 >>
         6230001 >>
    VOLUME OF SPIKING SOLUTION IN ML >>
```

(In this example, the numbers 6210001, 6220001, and 6230001 represent typical parameter-method codes. Non-Sample File Control users would find the names of the compounds in those positions.) Once again, you may supply spiking information for all of the spiked samples at once, or for groups of spiked samples, or for individual spiked samples by typing the appropriate sample wheel positions. If you have already provided dilution information for every one of the spiked samples in a group, the system does not need to ask for the volume of the sample.

---

*Default units are covered in Section 6.6.

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If the volume of your spiking solution is not significant, the system asks:

```
SPECIFY WHEEL POSITIONS OF SPIKES TO WHICH DATA APPLIES;
TYPE 0 (ZERO) AS A WHEEL POSITION TO END THE LIST

    FIRST POSITION >>
    LAST POSITION >>
    SAMPLE VOLUME IN ML >>
    MASS OF SPIKING COMPOUND IN DEFAULT MASS UNITS:*
        6210001 >>
        6220001 >>
        6230001 >>
```

If you have already provided dilution information for every one of the spiked samples in a group, the system does not need to ask for the volume of the samples. The default mass unit for the spiking compound is the numerator of the default concentration unit for the method. Thus, for a milligrams per liter method, use milligrams as the default mass unit; for a micrograms per liter method, use micrograms.

In either case, for samples which are to be diluted and spiked, always dilute before spiking. The laboratory automation project's standard procedures for these processes are discussed further in the paper, "Proposed Sample Dilution and Spiking Procedures for Sample File Control," by Dennis P. Ryan.[1]

6.4 ALLOWING FOR EXTRA REPEAT POSITIONS

During an automated run, if the system detects an offscale sample or if it encounters a sample for which it cannot determine the peak height, it automatically creates a repeat position for that sample at the end of the batch. However, you may allow "extra repeat positions" at the end of the batch for other samples which you may wish to remeasure.[2] The system asks:

```
WANT ANY EXTRA REPEAT POSITIONS ([N],Y) >>
```

and if you answer Y (yes), it asks:

```
HOW MANY EXTRA REPEAT POSITIONS >>
```

Any extra repeat positions you request are inserted into the sample wheel pattern before the last two blanks. You are not required to actually use any of the extra repeat positions you create, but their sample wheel positions should be filled with tubes of water if they are not used.

6.5 PRINTING THE SAMPLE WHEEL PATTERN

Before allowing you to print the sample wheel pattern, the system asks:

*Default units are covered in Section 6.6.

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NUMBER OF POSITIONS IN ONE SAMPLE WHEEL >>

From that point on, sample wheel positions are printed in the form

056 (2/016)

where, in this example, 056 is the position of the sample in the sample wheel pattern, and 2/016 indicates that this sample should be in the sixteenth position of the second forty-position sample wheel.

Next the system asks:

FORM OF SAMPLE WHEEL PATTERN REPORT ([H],L,T,B,N) >>

to allow you to get a copy of the complete sample wheel pattern on the lineprinter, the terminal, both, or neither. Figure 5 shows a sample wheel pattern report. On that report, the abbreviation "TCONC" stands for "theoretical concentration." "LSA" stands for "laboratory spike added value." The LSA value can be printed on the sample wheel pattern only for spikes where the volume of the spiking solution is not significant. The abbreviation "LCT" stands for "laboratory control standard theoretical concentration." LSA and LCT are standard Sample File Control data element abbreviations.[3]

6.6 PROVIDING VALUES FOR THE AUTOMATION PARAMETERS

The first time that you use the system, it forces you to supply all of the automation parameters, but on subsequent uses of the system, it asks:

AUTOMATION PARAMETERS ([H],A,U,) >>

where A means "accept the existing automation parameters," and U means "update the automation parameters." There are eleven automation parameter questions.

The first automation parameter is the default concentration unit for each analyte. The only choices allowed are milligrams per liter and micrograms per liter.

The second automation parameter is the time between peaks, in seconds. This must be exactly the same as the total cycle time of the automatic sampler. Decimal fractions of seconds are perfectly acceptable, if necessary.

The third automation parameter is whether or not you want a "subtracted results report." A subtracted results report is, for example, a report on the concentrations of nitrate in samples when the actual measured values were for nitrate-nitrite and nitrite. If you decide to have a subtracted results report, the system asks for the minuend analyte (the top number in the subtraction) and the subtrahend analyte (the bottom number in the subtraction).

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S-A-M-P-L-E W-H-E-E-L P-A-T-T-E-R-N
DATE: 05/02/80

WHEEL POSITION	SAMPLE TYPE	DILUTION FACTOR		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
001 (1/001)	SET STANDARD					
002 (1/002)	SET STANDARD					
003 (1/003)	SET STANDARD					
004 (1/004)	BLANK					
005 (1/005)	BLANK					
006 (1/006)	CAL STANDARD		TCONC:	30.000	15.000	20.000
007 (1/007)	CAL STANDARD		TCONC:	60.000	30.000	40.000
008 (1/008)	CAL STANDARD		TCONC:	90.000	45.000	60.000
009 (1/009)	BLANK					
010 (1/010)	BLANK					
011 (1/011)	ID: 00000001	1.00				
012 (1/012)	ID: 00000002	1.00				
013 (1/013)	SPIKE OF 012	1.00	LSA:	30.000	15.000	20.000
014 (1/014)	DUPE OF 012	1.00				
015 (1/015)	CONTROL STND		LCT:	45.000	22.500	30.000
016 (1/016)	CHECK OF 007					
017 (1/017)	REAGENT BLNK					
018 (1/018)	BLANK					
019 (1/019)	BLANK					
020 (1/020)	ID: 00000003	2.00				
021 (1/021)	ID: 00000004	2.00				
022 (1/022)	SPIKE OF 021	2.00	LSA:	30.000	15.000	20.000
023 (1/023)	DUPE OF 021	2.00				
024 (1/024)	CONTROL STND		LCT:	45.000	22.500	30.000
025 (1/025)	CHECK OF 007					
026 (1/026)	REAGENT BLNK					
027 (1/027)	ID: 00000005	1.00				
028 (1/028)	BLANK					
029 (1/029)	BLANK					
030 (1/030)	REPEAT OF [ ]	1.00				
031 (1/031)	REPEAT OF [ ]	1.00				
032 (1/032)	BLANK					
033 (1/033)	BLANK					

Figure 5. Sample Wheel Pattern Report.

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The fourth automation parameter is the dilution procedure for offscale samples. The choices are F (fixed dilution factor) or V (variable dilution factor). If you choose the fixed dilution factor option, you also have to provide your fixed dilution factor. Then during the automated run, if a sample is offscale, the system will tell you to dilute it by that factor and move it to a repeat position. Alternatively, if you choose the variable dilution factor procedure, the system will prescribe dilution factors for offscale samples, depending upon how far offscale they are. A prescribed dilution factor is always an integer, and should be enough to put the peak height of the sample within the range of the calibration standards.

The fifth automation parameter is the analogue to digital converter (A/D) channel number for each detector. The analogue to digital converter is the device which accepts the telemetry signal from the detector and uses it to generate a proportional number for the computer. The Nova system manager should have assigned you an analogue to digital converter channel number for each of your detectors.

The sixth automation parameter is the set standard threshold height, in percent of full scale, for each analyte. Timing set standards are solutions of known concentration which are the first samples in the batch. They should produce peaks of about 75% of full scale. Set standards are used by the system to synchronize itself with the automatic samplers. The threshold height is the parameter which enables the system to identify the first set standard. When you start the data acquisition process, the system begins to take readings from the analogue to digital converter, but it ignores them until they are higher than the threshold height you specify. It then takes readings from the first peak until the readings drop below the threshold height. Therefore, the threshold height must be low enough so that the first set standard will definitely go above it, but high enough so that the detector will definitely drop below it before the second peak comes along. Optimally, the threshold height should be chosen so that the peak is above it for the duration of a normal data acquisition window, as defined below.

The seventh automation parameter is the data acquisition window width, in seconds. The system does not pay attention to the detectors constantly. Instead, it takes readings only during data acquisition windows which bracket the times when the peaks pass over their summits. You should set the data acquisition window widths reasonably wide, but without allowing parts of adjacent peaks to show in the windows. Obviously, you must provide sufficient wash between samples to permit you to do this. The raw data plotting feature enables you to judge whether you have set the window widths appropriately, and whether you have allowed sufficient wash time between samples. Some experimentation with these parameters is probably necessary.

The eighth automation parameter is the standard deviation defining levelness, in percent of full scale, for each analyte. This system determines peak heights primarily by looking for the highest level position of each peak. Most peaks, however, do not have any perfectly level place. Therefore, to determine if a reading is on a level part of the peak, the system calculates the standard deviation of the five surrounding readings and determines whether it is less than the standarad deviation defining

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levelness. To ensure the accuracy of the peak height determination algorithm and the dependability of the timing synchronization algorithm, the standard deviation defining levelness should be set as low as possible. However, if this parameter is set too low, the system will reject good peaks. A setting of 5% is a very high value which can be used initially, and the raw data reporting features can be used to judge how much that value should be changed.

The ninth automation parameter is the degree of least squares regression for the calibration equation for each analyte. The choices are first degree, second degree, third degree, and linear interpolation (which is obviously not a form of regression). For a first degree regression, you must have at least two calibration standards, but to ensure the validity of your results, you should use at least three. For a second degree regression, you must have at least three standards, but it would be better to use at least four. For a third degree regression, you must have at least four standards, but it would be better to use at least five. At least two standards are required for linear interpolation. If you do not include enough calibration standards to perform the specified calibration, the system will terminate the automated run when it attempts to calibrate.

The tenth automation parameter is the detection limit, in default concentration units, for each analyte. The detection limit is the lowest calculated concentration which the system will report. Concentrations below the detection limit are shown on the reports and sent to Sample File Control as "BDL." It is permissible to set the detection limit absurdly low (even negative), in which case no results ever appear as BDL.

The eleventh automation parameter is the offscale concentration, in default concentration units, for each analyte. The offscale concentration is that concentration which the system will consider to be too high to report. In an attended run, the system instructs you to move offscale samples to repeat positions. Concentrations at or above the offscale concentration are shown on the reports as "OFFSCALE," and are transmitted to Sample File Control labeled "GTL" (greater than limit). It is permissible to set the offscale concentration absurdly high so that no samples ever go offscale.

After all of the automation parameters have been entered or updated, the system returns to the question:

AUTOMATION PARAMETERS ([H],A,U) >>

When you accept the automation parameters, the system advances to the next section.

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SECTION 7

ACQUIRING DATA

The peak height determination algorithms of this system are based on looking for the highest level place on each peak. A place is considered level if the standard deviation of five consecutive readings from the analogue to digital converter is less than the "standard deviation defining levelness" automation parameter. Plateaus at the tops of the peaks are desirable, but not at all essential. If an occasional peak does not go "up and over," the system reads its peak height from the "expected position of the most valid reading," which has been predicted on the basis of the most recent "up and over" peak. The reading from the expected position is not used unless it is at a place satisfying the definition of levelness. Timing synchronization between the system and the automatic sampler is maintained by advancing or retarding the data acquisition windows to keep the summits of the "up and over" peaks within the central third of the windows. Clearly, the reliability of the entire system is limited by how well your peaks conform to the system's expectations of what peaks should look like. Specifically, the sample to wash ratio of your automatic sampler must be low enough so that peaks are separate and distinct. The peak height determination and timing synchronization algorithms are discussed in detail in the document, "Functional Specifications for the Continuous Flow Analyzer Automation System,"[2] and they should be studied carefully.

7.1 FULL SCALE AND PROPER DAMPING

At the beginning of the data acquisition section, the CFA System instructs:

SET ALL DETECTORS TO FULL SCALE; THEN PRESS RETURN >>

and then:

SET ALL DETECTORS TO PROPER DAMPING; THEN PRESS RETURN >>

This procedure serves two purposes: 1) to check the hardware interface, and 2) to establish the baseline and full scale heights so that all of the peak heights can be reported as a percentage of the full scale deflection.

7.2 ATTENDED AND UNATTENDED RUNS

Next, the system asks:

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ATTENDED RUN ([N],Y) >>

The only difference between an attended run and an unattended run is that in an attended run the system instructs you to move offscale samples and samples whose peak heights cannot be determined to repeat positions, whereas in an unattended run, it does not.

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7.3 TIMING SET STANDARDS

Then, the system prompts:

PRESS 'RETURN' TO BEGIN DATA TAKING >>

Press the RETURN key just before the first timing set standard reaches the detector to start the real-time data acquisition process.

Figure 6 is an example of a progress report -- the report which is printed as the samples are measured. The data for each sample is reported after the peak for the slowest analyte is detected. For each timing set standard, the progress report shows the peak height (PH). The peak height is measured from the normal damping reading established earlier. For the first set standard, the peak height is reported only as "OK," since the system cannot always determine the peak height of the first peak accurately, even though it has successfully established timing synchronization with that peak.

7.4 BLANKS

For each blank, the progress report shows only the peak height (PH).

7.5 CALIBRATION STANDARDS

For each calibration standard, the progress report shows the baseline corrected peak height (BCPH) and the theoretical concentration (TCONC). The baseline corrected peak height is measured from the height of the most recent blank (or from the lower of the two most recent blanks where there are consecutive blanks).

Calibration

After the last calibration standard has been passed, the system performs calibration and reports the "calibration fitting error" and the "forced origin fitting error." Fitting error is a measure of how well the calibration curve fits the calibration data. It is calculated by the formula:

$$\text{Fitting Error} = \frac{100\sqrt{\frac{\sum(\text{Known conc.} - \text{Calc. conc.})^2}{\text{Number of standards} - \text{Degree} + 1}}}{\text{Mean conc.}}$$

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The "calibration fitting error" reflects the goodness of fit of the type of curve you selected. A fitting error of up to 5% would probably be

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(4-76)

P-R-O-G-R-E-S-S R-E-P-O-R-T
DATE: 05/02/80

WHEEL POSITION	SAMPLE TYPE	DILUTION FACTOR		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
001 (1/001)	SET STANDARD		PH:	OK	OK	OK
002 (1/002)	SET STANDARD		PH:	75.092	75.184	75.136
003 (1/003)	SET STANDARD		PH:	74.708	74.678	74.703
004 (1/004)	BLANK		PH:	1.671	1.689	1.720
005 (1/005)	BLANK		PH:	1.572	1.614	1.644
006 (1/006)	CAL STANDARD		BCPH:	29.968	29.946	29.951
			TCONC:	30.000	15.000	20.000
007 (1/007)	CAL STANDARD		BCPH:	58.260	58.215	58.217
			TCONC:	60.000	30.000	40.000
008 (1/008)	CAL STANDARD		BCPH:	86.981	86.936	86.903
			TCONC:	90.000	45.000	60.000
	CALIBRATION FITTING ERROR:			0.31%	0.00%	0.00%
	FORCED ORIGIN FITTING ERROR:			1.13%	1.12%	1.14%
	THE SECOND-TERMINAL CALIBRATION REPORT/PLOT IS NOW AVAILABLE					
009 (1/009)	BLANK		PH:	0.235	0.231	0.231
010 (1/010)	BLANK		PH:	0.158	0.171	0.172
011 (1/011)	ID: 00000001	1.00	BCPH:	59.789	59.766	59.775
			CONC:	61.458	30.816	41.086
012 (1/012)	ID: 00000002	1.00	BCPH:	40.546	40.555	40.549
			CONC:	41.286	20.657	27.499
013 (1/013)	SPIKE OF 012	1.00	BCPH:	69.288	69.192	69.198
			LSF:	71.371	35.762	47.658
			LSA:	30.000	15.000	20.000
			RECV:	100.54%	100.70%	100.76%
			QC:	OK	OK	OK
014 (1/014)	DUPE OF 012	1.00	BCPH:	41.899	41.879	41.962
			LD2:	42.632	21.368	28.498
			RNG:	1.424	0.703	0.999
			QC:	OK	OK	OK
015 (1/015)	CONTROL STND		BCPH:	44.264	44.292	44.385
			LCN:	45.120	22.642	30.213
			LCT:	45.000	22.500	30.000
			RECV:	100.27%	100.63%	100.71%
			QC:	OK	OK	OK
016 (1/016)	CHECK OF 007		BCPH:	59.582	59.450	59.476
			RECV:	102.13%	102.12%	102.16%
017 (1/017)	REAGENT BLNK		BCPH:	-0.438	-0.454	-0.140
			CONC:	-1.923	-1.392	-0.894
			QC:	OK	OK	OK
018 (1/018)	BLANK		PH:	-0.524	-0.461	-0.471
019 (1/019)	BLANK		PH:	-0.585	-0.574	-0.582
020 (1/020)	ID: 00000003	2.00	BCPH:	98.914	98.926	98.880
			CONC:	OFFSCALE	102.381	136.700
	DILUTE BY FACTOR OF 4.00 FOR TOTAL DILUTION OF 8.00; MOVE BLANK FROM WHEEL POSITION 032 (1/032) TO 034 (1/034); PLACE SAMPLE 00000003 IN WHEEL POSITION 032 (1/032)					
021 (1/021)	ID: 00000004	2.00	BCPH:	49.310	49.291	49.295
			CONC:	100.861	50.580	67.373
022 (1/022)	SPIKE OF 021	2.00	BCPH:	64.385	64.386	64.397
			LSF:	132.422	66.483	88.477
			LSA:	30.000	15.000	20.000
			RECV:	105.21%	105.49%	105.52%
			QC:	OK	OK	OK
023 (1/023)	DUPE OF 021	2.00	BCPH:	42.331	42.335	42.313
			LD2:	86.173	43.205	57.494
			RNG:	14.680	7.375	9.879
			QC:	UP CONT	UP CONT	UP CONT
	QC CONTROL LIMIT EXCEEDED					
024 (1/024)	CONTROL STND		BCPH:	42.838	41.987	42.837
			LCN:	42.778	21.418	28.551
			LCT:	45.000	22.500	30.000
			RECV:	95.06%	95.17%	95.17%
			QC:	OK	OK	OK
025 (1/025)	CHECK OF 007		BCPH:	52.958	52.902	52.943
			RECV:	90.98%	90.87%	90.94%
026 (1/026)	REAGENT BLNK		BCPH:	5.213	5.241	5.223
			CONC:	4.824	1.699	3.488
			QC:	OK	OK	OK
027 (1/027)	ID: 00000005	1.00	BCPH:	1.362	1.390	1.405
			CONC:	BDL	BDL	BDL
028 (1/028)	BLANK		PH:	0.783	0.735	0.785
029 (1/029)	BLANK		PH:	0.759	0.738	0.767
030 (1/030)	REPEAT OF [ ]	1.00	BCPH:	35.438	35.461	35.435
			CONC:	35.832	17.945	23.881
031 (1/031)	REPEAT OF [ ]	1.00	BCPH:	-0.452	-0.457	-0.453
			CONC:	BDL	BDL	BDL
032 (1/032)	REPEAT OF 020	8.00	BCPH:	47.608	47.638	47.604
			CONC:	389.120	195.319	259.925
033 (1/033)	BLANK		PH:	-2.210	-2.226	-2.210
034 (1/034)	BLANK		PH:	-2.210	-2.226	-2.210

Figure 6. Progress Report

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acceptable. Some analysts consistently achieve fitting errors of less than 1%. The "forced origin fitting error" measures how nearly your calibration points lie on a straight line passing through the origin. If forced origin fitting error is not an appropriate statistic for your analytical method, it can be ignored. It is included in the report for the benefit of analysts who use only the minimum number of calibration standards. For example, if you use second degree regression with only three calibration standards, the calibration fitting error will always be 0%, but the forced origin fitting error will indicate whether the calibration curve is reasonable or absurdly contorted. Forced origin regression is never used to calculate concentrations of samples; it is merely a double check on your selected regression.

When the calibration process is complete, the system prints:

THE SECOND TERMINAL CALIBRATION REPORT/PLOT IS NOW AVAILABLE

The use of that feature is described in Section 11 of this document.

7.6 UNKNOWNS

For each unknown, the progress report shows the baseline corrected peak height (BCPH) and the measured concentration (CONC). Dilution factors are taken into account in the measured concentration by use of the formula:

$$C_o = C_m \left(\frac{V_o + V_d}{V_o} \right)$$

where C_o is the calculated concentration of the original sample, C_m is the measured concentration of the diluted sample, V_o is the volume of the original sample, and V_d is the volume of the dilution water.

Peak heights which cannot be determined are reported as "CBD." Concentrations below the detection limit are reported as "BDL," and offscale concentrations are reported as "OFFSCALE."

Remeasurement Procedures

In an attended run, the system instructs you to move to a repeat position any unknown which must be remeasured. There are two such circumstances. For a sample in which any one of the analytes is offscale, the system instructs:

DILUTE BY FACTOR OF 4.00 FOR TOTAL DILUTION OF 24.00;
MOVE BLANK FROM WHEEL POSITION 075 (2/035) TO 077 (2/037);
PLACE SAMPLE 00000002 IN WHEEL POSITION 075 (2/035)

To dilute by a factor of D means to mix with water in a ratio of one part sample to D-1 parts water. For a sample for which the peak height for any one of the analytes cannot be determined, the system instructs:

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DO NOT DILUTE;
MOVE BLANK FROM WHEEL POSITION 076 (2/036) to 078 (2/038);
PLACE SAMPLE 00000003 IN WHEEL POSITION 076 (2/036)

In either case, the system rings the bell in the terminal four times to alert you to the message. If a sample contains one analyte which is offscale and another for which the peak height cannot be determined, the system calls for dilution. Similarly, if the system encounters one analyte which is both offscale and of undetermined peak height, the system calls for dilution. The procedure for moving blanks simply involves "leapfrogging" the second-last blank to the position after the last blank. This keeps two blanks at the end of the batch for baseline interpolation purposes. The system instructs you to move a sample only once. Thus, if an offscale sample is still offscale when it is remeasured, the system does not instruct you to dilute and move it again, since it is unlikely that you could get the rediluted sample into the proper wheel position in time for another remeasurement anyway. If any unknown involved in a quality control set has to be moved, no quality control assessment is made.

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7.7 SPIKED SAMPLES

For a spiked sample, the system reports the baseline corrected peak height (BCPH), the laboratory spike final concentration (LSA), the percent recovery (RECV), and the quality control assessment (QC). For undiluted samples spiked with an insignificant volume of spiking solution, the formula for LSA is:

$$LSA = \frac{M}{V_o}$$

where M is the mass of the analyte in the spiking solution and V_o is the volume of the sample. For undiluted samples spiked with a significant volume of spiking solution, the formula for LSA is:

$$LSA = \frac{C_s V_s - C_o V_s}{V_o + V_s}$$

where C_s is the concentration of the added spiking solution, V_s is the volume of the added spiking solution, C_o is the measured concentration of the original sample. For diluted samples which are spiked with insignificant volumes of spiking solution, the formula for LSA is the same as above, but for diluted samples spiked with a significant volume of spiking solution, the formula for LSA is:

$$LSA = \frac{C_s V_s V_o - C_m V_o V_s - C_m V_s V_d}{V_o V_o + V_o V_s}$$

where C_s is the concentration of the spiking solution, C_m is the measured concentration of the diluted but unspiked sample, V_s is the

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volume of the spiking solution, V_o is the volume of the undiluted, unspiked aliquot, and V_d is the volume of the dilution water. In addition, for the case of spiking a diluted sample with a significant volume of spiking solution, the formula for LSF becomes:

$$LSF = C_m \left(\frac{V_o + V_d + V_s}{V_o + V_s} \right)$$

where C_m is the measured concentration of the diluted, spiked sample, V_o is the volume of that sample before dilution, V_d is the volume of the dilution water, and V_s is the volume of the added spiking solution.

The percent recovery for the spike is always calculated by the formula:

$$\text{Percent Recovery} = \left(\frac{LSF - LSO}{LSA} \right) (100)$$

where LSO stands for "laboratory spike original concentration."

The quality control assessment for a spiked sample is made by comparing the percent recovery to the control limits supplied by Sample File Control or established during the creation of a non-Sample File Control run file. If the percent recovery is within the warning limits, the progress report shows a quality control assessment of "OK." The abbreviations "UP WARN" and "LOW WARN" indicate that the upper or lower warning limit has been exceeded. The system rings the bell in the terminal twice whenever a warning limit has been exceeded. The system rings the bell in the terminal three times whenever a control limit is exceeded, and it types the abbreviation "UP CONT" or "LOW CONT." The system never terminates an automated run because of an out of control situation; it is your decision whether or not to terminate the run by pressing ESCAPE.

7.8 DUPLICATES

For duplicates, the system reports the baseline corrected peak height (BCPH), the laboratory duplicate second member concentration (LD2), the range or absolute value of the difference between the measured concentrations (RNG), and the quality control assessment (QC). For samples having several duplicates, the duplicates are labeled LD3, LD4, LD5, etc. The quality control assessment for a duplicate is made by comparing the range to the "critical range" value which is calculated using the equation supplied by Sample File Control or established during the generation of a non-Sample File Control run file. If the range is less than the critical range, the quality control assessment is "OK," but if the range exceeds the critical range, the assessment is "UP CONT." The system rings the bell in the terminal three times whenever an "UP CONT" assessment occurs.

7.9 LABORATORY CONTROL STANDARDS

For a laboratory control standard, the progress report shows the

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baseline corrected peak height (BCPH), the laboratory control standard measured concentration (LCM), the laboratory control standard theoretical concentration (LCT), the percent recovery (RECV), and the quality control assessment. The percent recovery for a laboratory control standard is calculated by the formula:

$$\text{Percent Recovery} = \left(\frac{LCM}{LCT} \right) (100)$$

The quality control assessments for laboratory control standards are in the same form as those for spiked samples.

7.10 LABORATORY REAGENT BLANKS

For a laboratory reagent blank, the progress report shows the baseline corrected peak height (BCPH), the measured concentration (CONC), and the quality control assessment (QC). The concentration is always reported as calculated and never as "below detection limit." The quality control assessments for reagent blanks are in the same form as those for spiked samples, except that the judgments are made on the basis of concentration rather than percent recovery.

7.11 INSTRUMENT CHECK STANDARDS

For instrument check standards, the progress report shows the baseline corrected peak height (BCPH) and the percent recovery (RECV). The percent recovery for a check standard is calculated by the formula:

$$\text{Percent Recovery} = \left(\frac{\text{Peak height of check standard}}{\text{Peak height of calibration standard}} \right) (100)$$

The system also checks whether the percent recovery is within the allowable error which you set as an automation parameter. A lack of instrument stablility would be indicated by ringing the bell in the terminal three times and announcing:

ALLOWABLE ERROR FOR CHECK STANDARD EXCEEDED

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SECTION 8

MANIPULATING THE DATA

After data has been acquired and displayed on the progress report, the system gives you several opportunities to improve the accuracy of your results by manipulating the data.

8.1 BASELINE INTERPOLATION

The height of the baseline is automatically interpolated between the instrument blanks and subtracted from the peak heights of the intervening peaks. If you locate blanks in pairs in the sample wheel pattern, the system uses the lower of the two blanks in each pair as the endpoint of the interpolated baseline. The baseline height beneath a peak is estimated by the formula:

$$\text{Baseline Height} = \left(\frac{B_2 - B_1}{n + 1}\right) \quad (x) + (B_1)$$

where B_1 is the peak height of the blank before the interval, B_2 is the peak height of the blank after the interval, n is the number of samples in the interval (not counting the blanks on the ends), and x is the position of the sample in the interval.

This baseline drift compensation procedure is different from that in effect during the progress report, where the height of the baseline is simply taken as the height of the most recent blank (or the lower of the two in the most recent pair of blanks). Therefore, it is unlikely that the calculated results on the final report will ever exactly match those on the progress report, even if you do not use any of the other data manipulation features.

No interaction is required for baseline interpolation. While the system is interpolating the baseline, it prints:

THE BASELINE IS BEING INTERPOLATED.....

8.2 CALIBRATION INTERACTION

After baseline interpolation has been accomplished, the system recalibrates using the new baseline corrected peak heights for the calibration standards. As the system does this, it prints:

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THE FINAL CALIBRATION EQUATIONS ARE BEING DEVELOPED...
THE SECOND-TERMINAL CALIBRATION REPORT/PLOT IS NOW AVAILABLE

Next the system prompts:

CALIBRATION INTERACTION ([H],D,S,C,R,N) >>

where D stands for "display the calibration report/plot on this terminal," S stands for "suspend activity on this terminal while you get a second-terminal calibration report/plot," C stands for "change the degree of fit," R stands for "remove a calibration standard from consideration," and N stands for "none of the above."

If you choose to display the calibration report/plot on your current terminal, the system asks:

TERMINAL TYPE ([H],T,P,N) >>

where T stands for "Tektronix 4000 series computer display terminal," P stands for "Hewlett/Packard 2647 or 2648 terminal with Tektronix compatibility mode," and N stands for "neither of the above." If you have neither of the two graphics terminals, the system prints only the calibration report, including the table of residuals. On graphics terminals, the system prints the calibration report and draws the calibration curve, as shown in Figure 7. When the drawing of the curve is complete, the system rings the bell in the terminal four times, and then allows two minutes for you to make a hard copy. Pressing the RETURN key cuts short the two minute waiting period. After any calibration report/plot, the system returns to the calibration interaction menu.

If you choose to suspend activity on your current terminal while you get a second-terminal calibration report/plot, the system simply prompts:

PRESS 'RETURN' TO RESUME ACTIVITY ON THIS TERMINAL >>

Pressing RETURN sends you back to the calibration interaction menu. The use of the second-terminal report/plot feature is described in Section 11 of this document.

If you choose to change the degree of your least squares regression, the system again asks the degree of fit question of the automation parameters section. Any change you make at this point is permanent; that is, the new degree of fit will apply to all subsequent runs unless you change it again in the automation parameters section. After you have changed the degree of fit, the system reports:

THIS CHANGE IS BEING PROCESSED....
THE SECOND-TERMINAL CALIBRATION REPORT/PLOT IS NOW AVAILABLE

and then the system returns to the calibration interaction menu. You can always change the degree of fit and recalibrate again. Obviously, the

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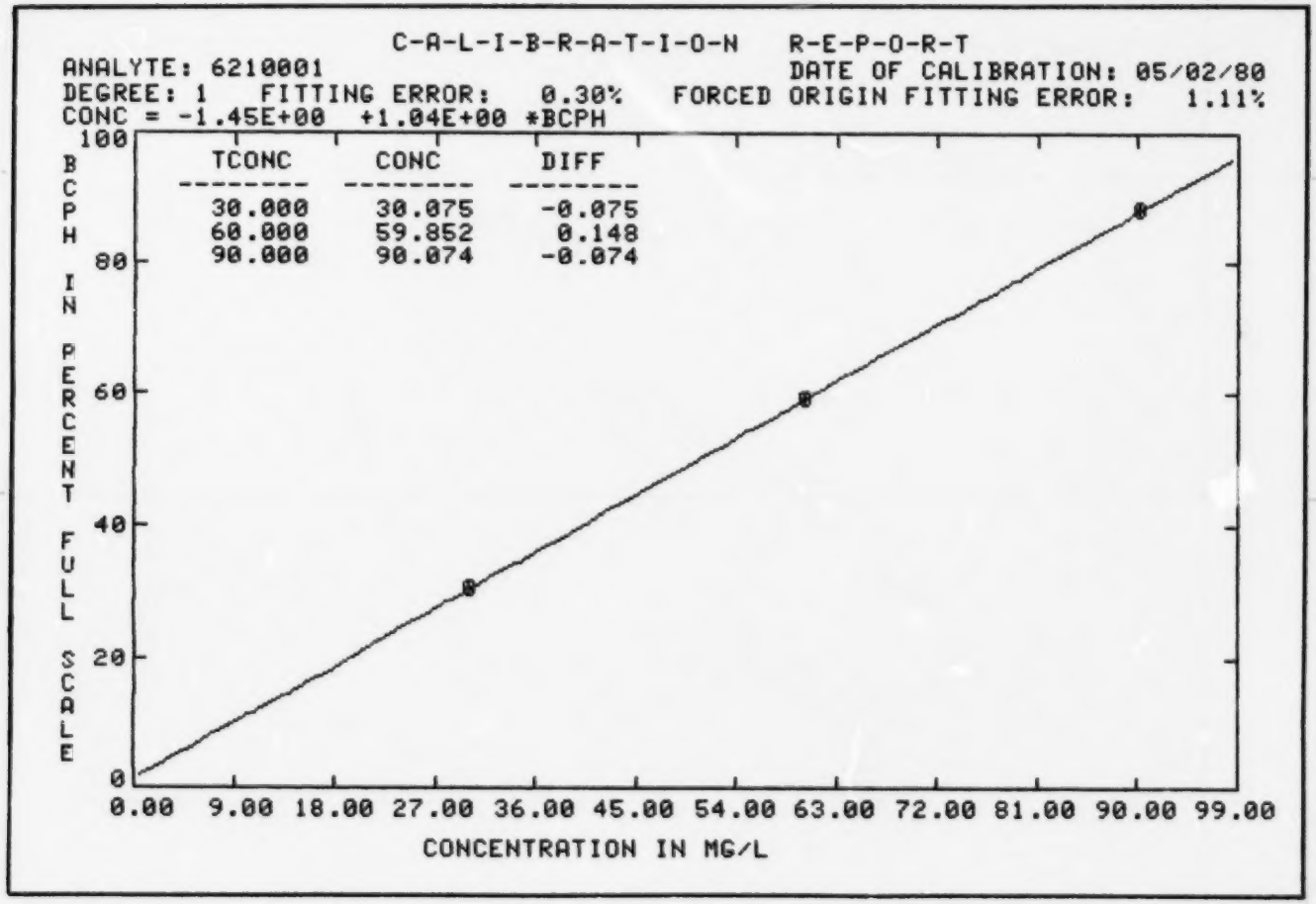

Figure 7. The Calibration Report/Plot.

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system cannot allow you to choose a degree of fit too high for the number of calibration standards in the batch.

If you choose to remove a calibration standard from consideration because it is an outlier, the system asks for the applicable analyte and the wheel position of the standard to be removed. The system recalibrates without the deleted standard and announces:

```
THIS CHANGE IS BEING PROCESSED...
THE SECOND-TERMINAL CALIBRATION REPORT/PLOT IS NOW AVAILABLE
```

The system cannot allow you to remove a standard if its removal would drop the number of standards below the minimum for the specified degree of fit. After the recalibration has been accomplished, the system returns to the calibration interaction menu. You may delete another standard at that point. There is one way to restore all of the standards you have removed from consideration; press ESCAPE to return to the CFA master command menu, choose the M (manipulate) option, and pass through the automatic baseline interpolation procedure again. This process restores all of the raw data to the way it was at the end of the data acquisition section.

When you choose the N option of the calibration interaction menu, the system advances to the next section. If you do not respond to the calibration interaction menu at all within ten minutes, the system assumes you want answer N, and it automatically advances to the next section.

8.3 REAGENT BLANK INTERACTION

If you have included any reagent blanks in your sample wheel pattern, the system asks:

```
REAGENT BLANK INTERACTION  ([H],D,S,N) >>
```

where D stands for "display a reagent blank report," S stands for "subtract reagent blank," and N stands for "neither of the above." If you type D, the system prints a report such as that shown in Figure 8. If you type S, the system asks:

```
SPECIFY WHEEL POSITIONS FROM WHICH REAGENT BLANK IS TO BE
SUBTRACTED;  TYPE 0 (ZERO) AS A WHEEL POSITION TO END THE LIST
     FIRST POSITION >>
     LAST POSITION >>
     VALUE TO BE SUBTRACTED FROM BCPH >>
```

As is apparent, this operation is not automatic, but it is totally flexible.

If you answer N to the reagent blank interaction question, the system advances to the next section. If you do not respond at all within two minutes, the system also advances to the next section. If you make a mistake in reagent blank subtraction, you can always return to the M (manipulate) option of the CFA master command menu to restore the data to its original form.

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8.4 EXTRA REPEAT POSITION INTERACTION

If you have included any extra repeat positions in your sample wheel pattern, the system asks:

```
EXTRA REPEAT POSITIONS INTERACTION  ([H],D,I,N) >>
```

where D stands for "display an extra repeat positions report," I stands for "identify extra repeat positions," and N stands for "neither of the above." If you type D, the system prints a report such as that shown in Figure 9. If you choose to identify one of the repeat positions, the system asks:

```
WHEEL POSITION OF EXTRA REPEAT >>
ORIGINAL WHEEL POSITION OF SAMPLE >>
DILUTION INFORMATION:
     SAMPLE VOLUME IN ML >>
     DILUTION WATER VOLUME IN ML >>
```

These questions allow you to dilute a sample when you move it to an extra repeat position.

If you answer N to the extra repeat positions interaction question, the system advances to the next section. If you do not respond at all within two minutes, the system automatically advances to the next section.

8.5 THE FINAL REPORT

When all of the data manipulation has been completed, the systems asks:

```
FORM OF FINAL REPORT  ([H],L,T,B,N) >>
```

where L stands for "lineprinter," T stands for "terminal," B stands for "both lineprinter and terminal," and N stands for "neither lineprinter nor terminal." If you do not respond to this question within two minutes, the system assumes that you want the report to be printed on the lineprinter. The system then provides the option:

```
DETAILED HEADING INFORMATION  ([N],Y) >>
```

Answering Y (yes) to this question causes the system to include the automation parameters at the top of the final report, as they are in Figure 10. If you request the detailed heading information, the system also provides the opportunity:

```
COMMENTS ([NONE],---) >>
```

in which you may type any sixty characters (no commas allowed).

8.6 THE SUBTRACTED RESULTS REPORT

If you specified a subtracted results report in the automation parameters section, the system asks at this point:

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R-E-A-G-E-N-T B-L-A-N-K R-E-P-O-R-T
DATE: 05/02/80

WHEEL POSITION	SAMPLE TYPE	DILUTION FACTOR		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
006 (1/006)	CAL STANDARD		BCPH:	30.302	30.292	30.304
			TCONC:	30.000	15.000	20.000
007 (1/007)	CAL STANDARD		BCPH:	58.929	58.907	58.924
			TCONC:	60.000	30.000	40.000
008 (1/008)	CAL STANDARD		BCPH:	87.983	87.973	87.963
			TCONC:	90.000	45.000	60.000
015 (1/015)	CONTROL STND		BCPH:	44.693	44.694	44.794
			LCT:	45.000	22.500	30.000
017 (1/017)	REAGENT BLNK		BCPH:	0.159	0.101	0.426
024 (1/024)	CONTROL STND		BCPH:	41.193	41.156	41.172
			LCT:	45.000	22.500	30.000
026 (1/026)	REAGENT BLNK		BCPH:	4.106	4.171	4.108

9-1/8"

Figure 8. The Reagent Blank Report.

E-X-T-R-A R-E-P-E-A-T P-O-S-I-T-I-O-N-S R-E-P-O-R-T
DATE: 05/02/80

WHEEL POSITION	SAMPLE TYPE	DILUTION FACTOR		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
030 (1/030)	REPEAT OF [ ]		BCPH:	36.612	36.641	36.615
031 (1/031)	REPEAT OF [ ]		BCPH:	1.320	1.314	1.325

Figure 9. The Extra Repeat Positions Report.

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F-I-N-A-L R-E-P-O-R-T
DATE: 05/02/80

COMMENTS: SIMULATED THREE-ANALYTE RUN
NAME OF RUN FILE: 6200001.RF
MODE OF OPERATION: ATTENDED
TIME BETWEEN PEAKS: 30 SECONDS
ADDITIONAL DILUTION FACTOR FOR OFFSCALE SAMPLES: 4

	6210001 VALUES	6220001 VALUES	6230001 VALUES
DEFAULT CONCENTRATION UNIT:	MG/L	MG/L	MG/L
A/D CHANNEL NUMBER:	10	11	10
SET STANDARD THRESHOLD HEIGHT:	50	50	50
DATA ACQUISITION WINDOW WIDTH:	20	20	20
STANDARD DEVIATION DEFINING LEVELNESS:	0.60	0.60	0.60
DETECTION LIMIT:	20.000	12.000	18.000
OFFSCALE CONCENTRATION:	90.000	95.000	95.000
ALLOWABLE ERROR FOR CHECK STANDARDS:	10.00%	10.00%	10.00%
TYPE OF FIT:	1	2	0
CALIBRATION FITTING ERROR:	0.78%	0.00%	0.00%
FORCED ORIGIN FITTING ERROR:	1.11%	1.10%	1.12%

CALIBRATION EQUATIONS:
6210001: CONC = -1.45E+00 +1.04E+00 *BCPH
6220001: CONC = -1.13E+00 +5.37E-01 *BCPH -1.41E-04 *BCPH^2
6230001: INTERPOLATION

WHEEL POSITION	SAMPLE TYPE	DILUTION FACTOR		6210001 RESULTS	6220001 RESULTS	6230001 RESULTS
001 (1/001)	SET STANDARD		PH:	100.013	CBD	99.997
002 (1/002)	SET STANDARD		PH:	75.092	75.184	75.136
003 (1/003)	SET STANDARD		PH:	74.708	74.678	74.703
004 (1/004)	BLANK		PH:	1.671	1.689	1.720
005 (1/005)	BLANK		PH:	1.572	1.614	1.644
006 (1/006)	CAL STANDARD		BCPH:	38.382	38.292	38.314
			TCONC:	30.000	15.000	20.000
007 (1/007)	CAL STANDARD		BCPH:	58.929	58.907	58.924
			TCONC:	60.000	30.000	40.000
008 (1/008)	CAL STANDARD		BCPH:	87.983	87.973	87.963
			TCONC:	90.000	45.000	60.000
009 (1/009)	BLANK		PH:	0.235	0.231	0.231
010 (1/010)	BLANK		PH:	0.158	0.171	0.172
011 (1/011)	ID: 00000001	1.00	BCPH:	59.881	SEE 030	SEE 030
			CONC:	60.842		
012 (1/012)	ID: 00000002	1.00	BCPH:	40.722	40.726	40.724
			CONC:	40.913	26.496	27.282
013 (1/013)	SPIKE OF 012	1.00	BCPH:	69.468	69.448	69.444
			LSF:	70.015	35.463	47.245
			LSA:	30.000	15.000	20.000
			RECV:	99.67%	99.78%	99.82%
			QC:	OK	OK	OK
014 (1/014)	DUPE OF 012	1.00	BCPH:	42.244	42.243	42.293
			LD2:	42.496	21.272	26.378
			RMS:	1.583	0.776	1.096
			QC:	OK	OK	OK
015 (1/015)	CONTROL STND		BCPH:	44.693	44.694	44.794
			LCN:	45.044	22.578	30.126
			LCT:	45.000	22.500	30.000
			RECV:	100.16%	100.35%	100.42%
			QC:	OK	OK	OK
016 (1/016)	CHECK OF 007		BCPH:	60.815	59.929	59.964
			RECV:	101.84%	101.73%	101.77%
017 (1/017)	REAGENT BLNK		BCPH:	0.159	0.181	0.426
			CONC:	-1.288	-1.076	0.281
			QC:	OK	OK	OK
018 (1/018)	BLANK		PH:	-0.524	-0.461	-0.471
019 (1/019)	BLANK		PH:	-0.595	-0.574	-0.582
020 (1/020)	ID: 00000003	2.00	BCPH:	SEE 032	98.573	98.518

021 (1/021)	ID: 00000004	2.00	CONC:		100.822	134.539
			BCPH:	48.856	48.819	48.887
022 (1/022)	SPIKE OF 021	2.00	CONC:	98.748	49.476	65.861
			BCPH:	63.721	63.714	63.684
			LSF:	129.672	64.995	86.557
			LSA:	30.000	15.000	20.000
			RECV:	103.80%	103.46%	103.48%
			QC:	OK	OK	OK
023 (1/023)	DUPE OF 021	2.00	BCPH:	41.616	41.623	41.575
			LD2:	83.606	41.935	55.752
			RMS:	15.862	7.541	10.108
			QC:	UP CONT	UP CONT	UP CONT
024 (1/024)	CONTROL STND		BCPH:	41.193	41.156	41.172
			LCN:	41.463	20.722	27.595
			LCT:	45.000	22.500	30.000
			RECV:	92.01%	92.10%	91.98%
			QC:	OK	OK	OK
025 (1/025)	CHECK OF 007		BCPH:	51.981	51.952	51.953
			RECV:	88.21%	88.17%	88.17%
026 (1/026)	REAGENT BLNK		BCPH:	4.186	4.171	4.188
			CONC:	2.826	1.106	2.711
			QC:	OK	OK	OK
027 (1/027)	ID: 00000005	1.00	BCPH:	0.124	0.200	0.164
			CONC:	BBL	BBL	BBL
028 (1/028)	BLANK		PH:	0.703	0.735	0.705
029 (1/029)	BLANK		PH:	0.759	0.738	0.767
THE FOLLOWING RESULTS ARE SIGNIFICANT ONLY AS INDICATED ABOVE:						
030 (1/030)	REPEAT OF 011	1.00	BCPH:	36.612	36.641	36.615
			CONC:	36.637	18.348	24.418
031 (1/031)	REPEAT OF [ ]	1.00	BCPH:	1.320	1.314	1.325
			CONC:	BBL	BBL	BBL
032 (1/032)	REPEAT OF 020	0.00	BCPH:	49.979	50.002	49.992
			CONC:	484.337	242.051	278.869
033 (1/033)	BLANK		PH:	-2.210	-2.224	-2.210
034 (1/034)	BLANK		PH:	-2.210	-2.226	-2.210

Figure 10. The Final Report.

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FORM OF SUBTRACTED RESULTS REPORT ([H],L,T,B,N) >>

where the letters represent the same options as before. If you do not answer the question within two minutes, the system assumes you want the report to be printed on the lineprinter. Figure 11 shows a subtracted results report.

After all of the reports have been printed, the system advances to the next section if you started with a run file from the Sample File Control System, or it returns to the CFA master command menu if you started with a non-Sample File Control run file. If you think the accuracy of the results on the final report could be improved by remanipulating the data, you can always use the M (manipulate) option of the CFA master command menu, as described before.

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S-U-B-T-R-A-C-T-E-D R-E-S-U-L-T-S R-E-P-O-R-T
DATE: 05/02/80

WHEEL POSITION	SAMPLE TYPE	DILUTION FACTOR		6210001 RESULTS	6220001 RESULTS	DIFFERENCE
011 (1/011)	ID: 00000001	1.00	CONC:	60.842	SEE 030	42.494
012 (1/012)	ID: 00000002	1.00	CONC:	40.913	20.496	20.417
020 (1/020)	ID: 00000003	2.00	CONC:	SEE 032	100.822	303.514
021 (1/021)	ID: 00000004	2.00	CONC:	98.748	49.476	49.272
027 (1/027)	ID: 00000005	1.00	CONC:	BDL	BDL	CBD
THE FOLLOWING RESULTS ARE SIGNIFICANT ONLY AS INDICATED ABOVE:						
030 (1/030)	REPEAT OF 011	1.00	CONC:	36.637	18.348	
031 (1/031)	REPEAT OF [ ]	1.00	CONC:	BDL	BDL	
032 (1/032)	REPEAT OF 020	8.00	CONC:	404.336	202.851	

Figure 11. The Subtracted Results Report.

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SECTION 9

FILLING THE SAMPLE FILE CONTROL RUN RESULTS FILE

Filling the Sample File Control run results file is a completely automatic process which requires only that you approve the results by answering Y (yes) to the question:

APPROVE RESULTS TO FILL SFC RUN RESULTS FILE ([N],Y) >>

After the run results file has been filled, the system gives you the opportunity to print the contents of that file by asking the question:

6-1/2"

FORM OF RUN RESULTS FILE REPORT ([H],L,T,B,N) >>

where the letters stand for the same options as for other reports. It is unlikely that you will want to print this report. A typical run results file report is shown in Figure 12.

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```
1 80 05 02 12 33 IIII  000YZNN III
3                P   6210001 +1.000E+02 T
3                P   6220001            T
3                P   6230001 +1.000E+02 T
3                P   6210001 +7.509E+01 T
3                P   6220001 +7.510E+01 T
3                P   6230001 +7.514E+01 T
3                P   6210001 +7.470E+01 T
3                P   6220001 +7.468E+01 T
3                P   6230001 +7.470E+01 T
3                P   6210001 +1.671E+00 B
3                P   6220001 +1.689E+00 B
3                P   6230001 +1.720E+00 B
3                P   6210001 +1.572E+00 B
3                P   6220001 +1.614E+00 B
3                P   6230001 +1.644E+00 B
3   +3.000E+01   P   6210001 +3.030E+01 S
3   +1.500E+01   P   6220001 +3.029E+01 S
3   +2.000E+01   P   6230001 +3.030E+01 S
3   +6.000E+01   P   6210001 +5.893E+01 S
3   +3.000E+01   P   6220001 +5.891E+01 S
3   +4.000E+01   P   6230001 +5.892E+01 S
3   +9.000E+01   P   6210001 +8.798E+01 S
3   +4.500E+01   P   6220001 +8.797E+01 S
3   +6.000E+01   P   6230001 +8.796E+01 S
3                P   6210001 +2.346E-01 B
3                P   6220001 +2.309E-01 B
3                P   6230001 +2.314E-01 B
3                P   6210001 +1.579E-01 B
3                P   6220001 +1.709E-01 B
3                P   6230001 +1.723E-01 B
6 00000001 003   P   000YZNN
2 00000001       P   6210001 +6.084E+01 MG/L
2 00000001       P   6220001 +1.835E+01 MG/L
2 00000001       P   6230001 +2.441E+01 MG/L
6 00000002 003   P   000YZNN
2 00000002 LDX   P   6210001 +4.091E+01 MG/L
4 LSPK     UCL   P   6210001 +1.150E+02 00/00/00
4 LSPK     UWL   P   6210001 +1.100E+02 00/00/00
4 LSPK     AVE   P   6210001 +1.000E+02 00/00/00
4 LSPK     LWL   P   6210001 +9.000E+01 00/00/00
4 LSPK     LCL   P   6210001 +8.500E+01 00/00/00
4 LDUP     A     P   6210001 +0.000E+00 00/00/00
4 LDUP     B     P   6210001 +0.000E+00 00/00/00
4 LDUP     C     P   6210001 +1.500E-01 00/00/00
4 LDUP     D     P   6210001 +0.000E+00 00/00/00
2 00000002 LDX   P   6220001 +2.050E+01 MG/L
4 LSPK     UCL   P   6220001 +1.150E+02 00/00/00
4 LSPK     UWL   P   6220001 +1.100E+02 00/00/00
4 LSPK     AVE   P   6220001 +1.000E+02 00/00/00
4 LSPK     LWL   P   6220001 +9.000E+01 00/00/00
4 LSPK     LCL   P   6220001 +8.500E+01 00/00/00
4 LDUP     A     P   6220001 +0.000E+00 00/00/00
4 LDUP     B     P   6220001 +0.000E+00 00/00/00
4 LDUP     C     P   6220001 +1.500E-01 00/00/00
4 LDUP     D     P   6220001 +0.000E+00 00/00/00
2 00000002 LDX   P   6230001 +2.728E+01 MG/L
4 LSPK     UCL   P   6230001 +1.150E+02 00/00/00
4 LSPK     UWL   P   6230001 +1.100E+02 00/00/00
4 LSPK     AVE   P   6230001 +1.000E+02 00/00/00
4 LSPK     LWL   P   6230001 +9.000E+01 00/00/00
4 LSPK     LCL   P   6230001 +8.500E+01 00/00/00
4 LDUP     A     P   6230001 +0.000E+00 00/00/00
4 LDUP     B     P   6230001 +0.000E+00 00/00/00
4 LDUP     C     P   6230001 +1.500E-01 00/00/00
4 LDUP     D     P   6230001 +0.000E+00 00/00/00
```

Figure 12. The Run Results File Contents.

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SECTION 10

CHECKING THE INTERFACE

To check the interface between your instrument and the computer, you can use the C (check) option of the CFA master command menu. Under this option, the system simply asks:

A/D CHANNEL TO BE TESTED >>

It then prints the analogue to digital converter readings for that channel until you press ESCAPE or until 720 readings have been printed. The analogue to digital coverter readings should parallel the activity on your recorder if all of the interface hardware and software is functioning properly. At proper damping, the readings should be roughly 400. At full scale, the readings should be roughly 8200.

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SECTION 11

DISPLAYING THE RAW DATA

Two of the automation parameters -- data acquisition window width and standard deviation defining levelness -- must be "fine tuned" for each analyte during the first few uses of the system. The raw data reporting and plotting features enable you to judge how well you have set these parameters. When you choose the D (display) option of the CFA master command menu, you reach the question:

MODE OF RAW DATA DETAILS ([H],P,R,) >>

where P stands for "plot of peaks," and R stands for "report of raw data."

11.1 THE RAW DATA PLOT

If you choose to plot raw data, the system asks for the type of terminal, the first and last wheel positions to be included, and (in multi-analyte batches) the analyte of interest. No more than ten peaks can be plotted at a time. As mentioned previously, plotting can only be done on a Tektronix terminal or a Hewlett-Packard terminal with Tektronix compatibility mode. Figure 13 shows a typical peak plot. You can use such a plot to judge whether you have set the data acquisition window width properly. Ideally, each window should show both the rising and falling sides of a peak, without showing the bottoms of valleys between peaks or parts of adjacent peaks.

11.2 THE RAW DATA REPORT

Figure 14 shows a typical raw data report. To get such a report, you must answer questions regarding the first and last wheel positions to be included, the form of the report, and the analyte of interest. Because the raw data reports are rather long, the system does not allow you to create such a report for more than ten peaks at a time. When sending such report to the lineprinter, remember that a set of raw data reports for 200 samples measured for three analytes would cover over 700 sheets of paper.

The raw data reports enable you to judge how well you have set the standard deviation defining levelness. For each peak, find the highest "smoothed reading," and note the standard deviation at that position. Determine what would have been the smallest standard deviation defining levelness which would have not eliminated any of your legitimate peaks. Experiment with that value in the next run, and adjust it until the system accepts those peaks which you consider legitimate and rejects those peaks which you consider "noisy."

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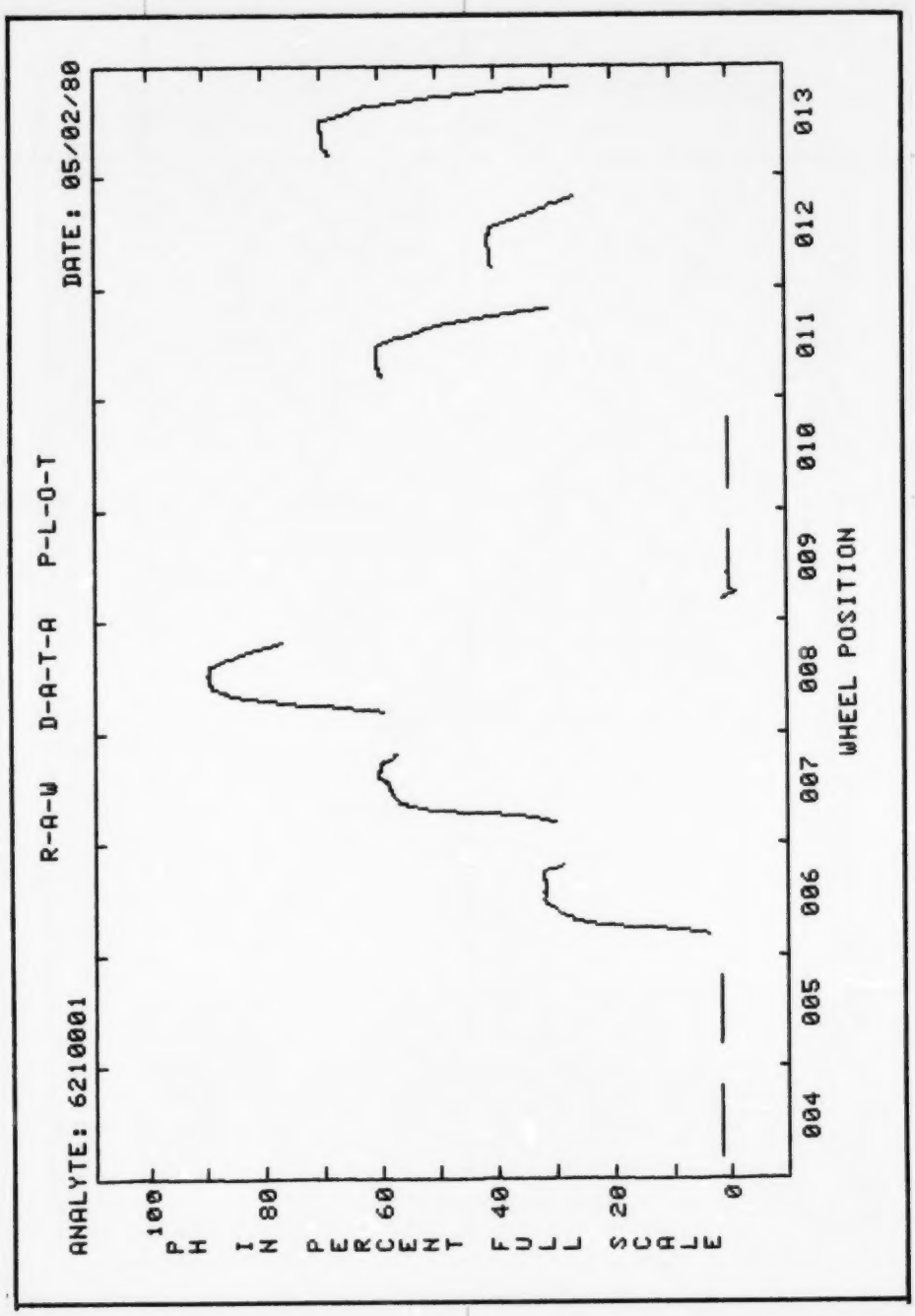

Figure 13. The Raw Data Plot.

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R-A-W D-A-T-A R-E-P-O-R-T
DATE: 05/02/80

ANALYTE: 6210001

WHEEL POSITION: 8
PEAK HEIGHT: 88.552
HIGHEST LEVEL POSITION: 33
EXPECTED POSITION: 32

ALGORITHM APPLIED: HIGHEST LEVEL POSITION
TIMING ADJUSTMENT: NONE
HEIGHT AT HIGHEST LEVEL POSITION: 88.552
HEIGHT AT EXPECTED POSITION: 88.545

READING NUMBER	RAW READING	SMOOTHED READING	STANDARD DEVIATION
1	58.794		
2	60.717		
3	63.159	63.001	3.016
4	64.819	64.703	3.227
5	66.236	66.498	3.843
6	69.299	69.357	4.299
7	72.837	72.645	4.116
8	75.004	74.869	3.452
9	76.189	76.553	2.569
10	78.356	77.957	2.432
11	79.214	79.523	2.566
12	81.131	81.085	2.297
13	82.868	82.723	2.180
14	83.727	83.854	1.637
15	84.701	84.653	1.127
16	85.297	85.280	0.835
17	85.579	85.533	0.767
18	85.810	85.941	1.027
19	86.790	86.805	1.081
20	87.790	87.646	0.928
21	87.906	87.952	0.509
22	87.912	87.941	0.149
23	88.040	88.038	0.156
24	88.181	88.169	0.164
25	88.252	88.255	0.137
26	88.316	88.328	0.092
27	88.399	88.377	0.069
28	88.386	88.403	0.048
29	88.418	88.411	0.043
30	88.444	88.450	0.059
31	88.495	88.491	0.063
32	88.534	88.545	0.048
33	88.572	88.552	0.057
34	88.495	88.502	0.082
35	88.418	88.422	0.092
36	88.373	88.373	0.065
37	88.348	88.348	0.038
38	88.335	88.342	0.062
39	88.322	88.343	0.289
40	88.213	88.150	0.543
41	87.668	87.678	0.687
42	87.085	87.141	0.752
43	86.752	86.713	0.709
44	86.303	86.320	0.750
45	85.823	85.815	0.931
46	85.194	85.1[illegible]	[illegible]
47	84.387	[illegible]	
48	83.970		
49	87[illegible]		
50			

Figure 14. The Raw Data Report.

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SECTION 12

PLOTTING THE CALIBRATION CURVES DURING AN AUTOMATED RUN

The second-terminal calibration report/plot feature enables you to log on to the computer through a second terminal and get the details of your calibration while the system continues to acquire data and print the progress report on your first terminal. It also allows users who must share a graphics terminal to suspend activity on their own terminals after recalibratiion, go to the shared graphics terminal to see their calibration curves, and then resume activity on their main terminals.

To use this feature, simply log on to the computer through a second terminal using the second account ID for the current analyte. The system asks for the type of terminal and (in a multi-analyte batch) the name of the analyte of interest. It then prints a report including the table of residuals, and on a Tektronix or Tektronix compatible terminal, it draws the plot of the curve, as shown in Figure 7.

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SECTION 13

NOTES TO THE SYSTEM MANAGER

The Continuous Flow Analyzer (CFA) Automation System consists of 21 programs named CFA00 through CFA20 and seven data files named CFA000 through CFA006.4 The CFA system can also produce a non-Sample File Control run file named 0000000.RF.

The system is designed to run in a shared directory with two account IDs -- one for access to the main group of programs and a second for access to the "second terminal calibration report/plot" program. The listing in BASIC.ID for the first account ID should send the user to the message of the day program in the BASIC library, which should then chain to the Sample File Control INITIALIZE program. INITIALIZE must chain to the program named AUTORUN which must be resident in the user's directory, and which must contain the statement

```
CHAIN"CFA00"
```

If the user is not involved in Sample File Control, it would be possible for the message of the day program to chain directly to AUTORUN. However, in such a case, there would have to be a program named INITIALIZE in the user's directory containing the statement

```
BYE
```

to enable the CFA System to log off from the computer.

The listing in BASIC.ID for the second account ID should send the user to a second message of the day program in the BASIC library, which must then chain to a program named INITIALIZE.2 in the user's directory. INITIALIZE.2 must contain the statement

```
CHAIN"CFA20"
```

To use the second terminal calibration report/plot feature, the users will need to have access to a Tektronix 4000 Series Computer Display Terminal or a Hewlett-Packard 2647 or 2648 terminal with Tektronix compatibility mode.

All of the programs other than AUTORUN and INITIALIZE.2 (and the "BYE-only" version of INITIALIZE) can be kept in the BASIC library.

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The users should be provided with separate directories for each analyte or group of analytes which are regularly measured. The shared directories must be INITed and never RELEASEd from the background console. If this is not done, logging off from either of the account ID's will result in the other account ID experiencing UNKNOWN DIR SPECIFIER errors.

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2. Kopke, Jonathan E. Functional Specifications for the Continuous Flow Analyzer Automation System, 1980. EPA Report to be published.

3. Initial Data Element Dictionary (DED) for the Sample File Control (SFC) System, Auerback Associates, Inc., 1978.

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